



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2014 – 01:16 PM EDT

PDB ID : 3WCJ  
Title : The complex structure of HsSQS wtih ligand,E5700  
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;  
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Deposited on : 2013-05-27  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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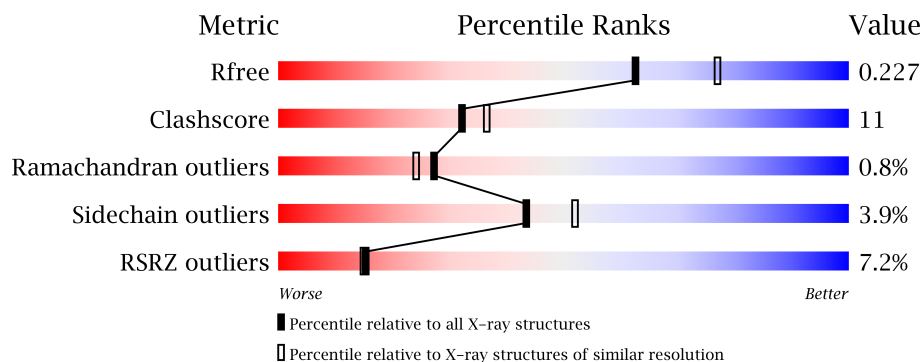
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	
1	E	360	
1	F	360	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17199 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	B	332	Total	C	N	O	S	0	0	0
			2678	1705	453	502	18			
1	C	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	D	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	E	335	Total	C	N	O	S	0	0	0
			2704	1721	460	505	18			
1	F	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			

There are 23 discrepancies between the modelled and reference sequences:

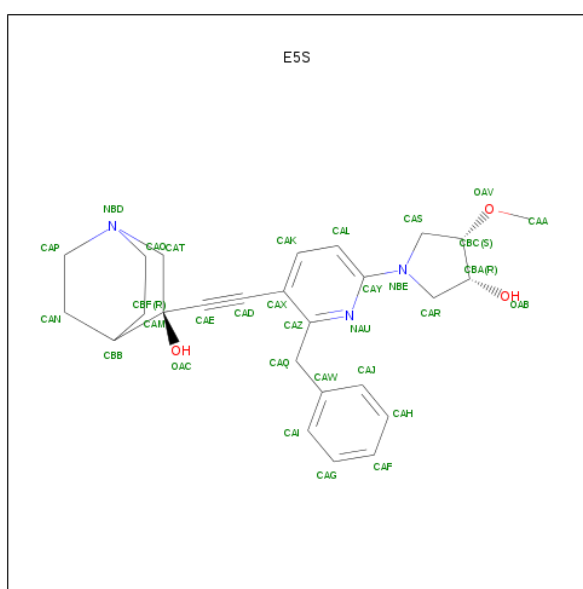
Chain	Residue	Modelled	Actual	Comment	Reference
A	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	353	ASN	ASP	SEE REMARK 999	UNP P37268
B	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
B	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
B	353	ASN	ASP	SEE REMARK 999	UNP P37268
C	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	353	ASN	ASP	SEE REMARK 999	UNP P37268
D	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	353	ASN	ASP	SEE REMARK 999	UNP P37268
E	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
E	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
E	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
E	353	ASN	ASP	SEE REMARK 999	UNP P37268
F	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
F	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
F	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
F	353	ASN	ASP	SEE REMARK 999	UNP P37268

- Molecule 2 is (3R)-3-( $\{2\text{-BENZYL-6-}[(3R,4S)\text{-3-HYDROXY-4-METHOXYPIRROLIDIN-1-YL}]\text{PYRIDIN-3-YL}\}$ ETHYNYL)-1-AZABICYCLO[2.2.2]OCTAN-3-OL (three-letter code: E5S) (formula:  $\text{C}_{26}\text{H}_{31}\text{N}_3\text{O}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	26	3	3		
2	B	1	Total	C	N	O	0	0
			32	26	3	3		
2	C	1	Total	C	N	O	0	0
			32	26	3	3		
2	D	1	Total	C	N	O	0	0
			32	26	3	3		
2	E	1	Total	C	N	O	0	0
			32	26	3	3		
2	F	1	Total	C	N	O	0	0
			32	26	3	3		

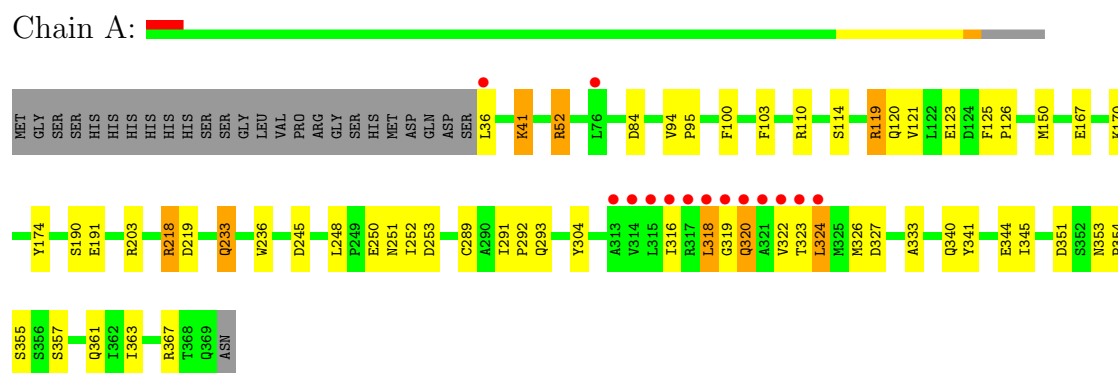
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total 178	O 178	0	0
3	B	204	Total 204	O 204	0	0
3	C	160	Total 160	O 160	0	0
3	D	131	Total 131	O 131	0	0
3	E	86	Total 86	O 86	0	0
3	F	66	Total 66	O 66	0	0

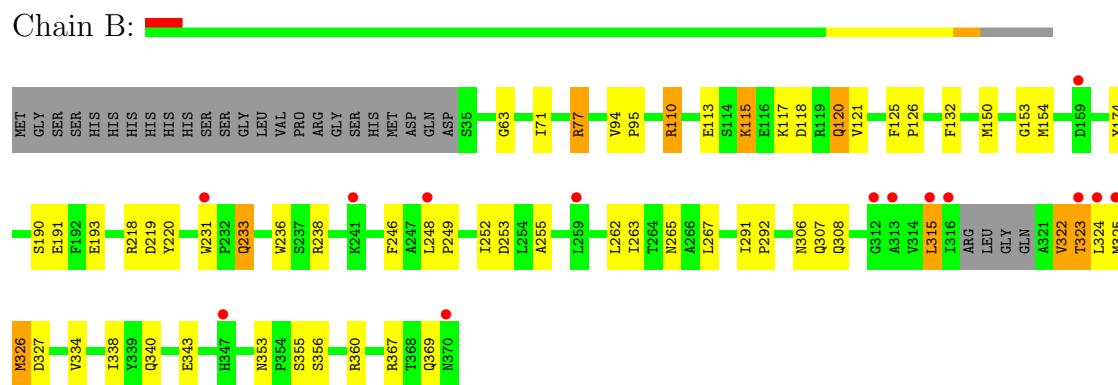
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

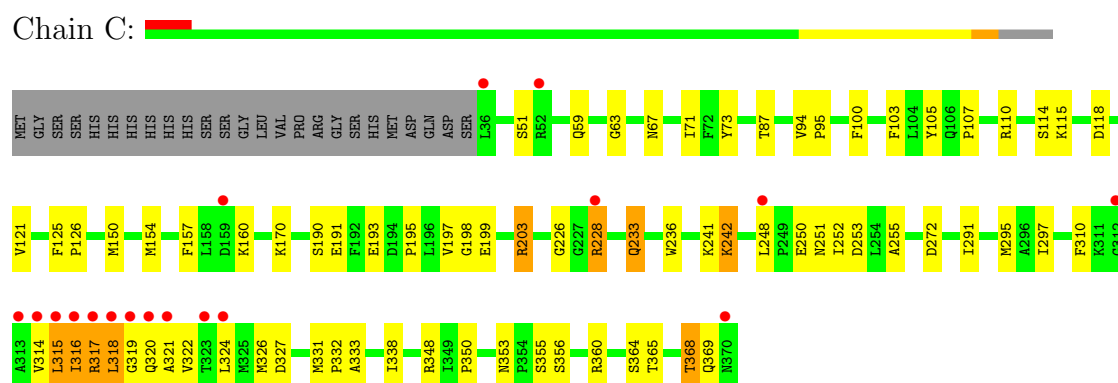
- Molecule 1: Squalene synthase



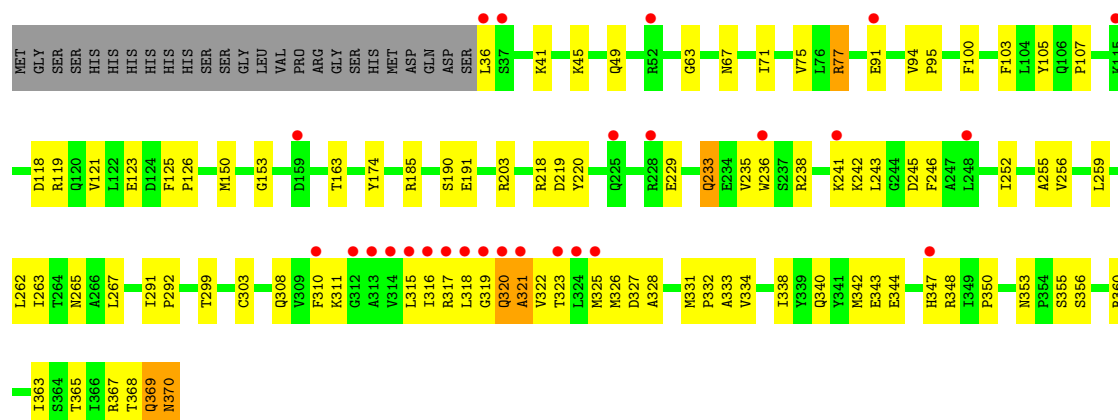
- Molecule 1: Squalene synthase



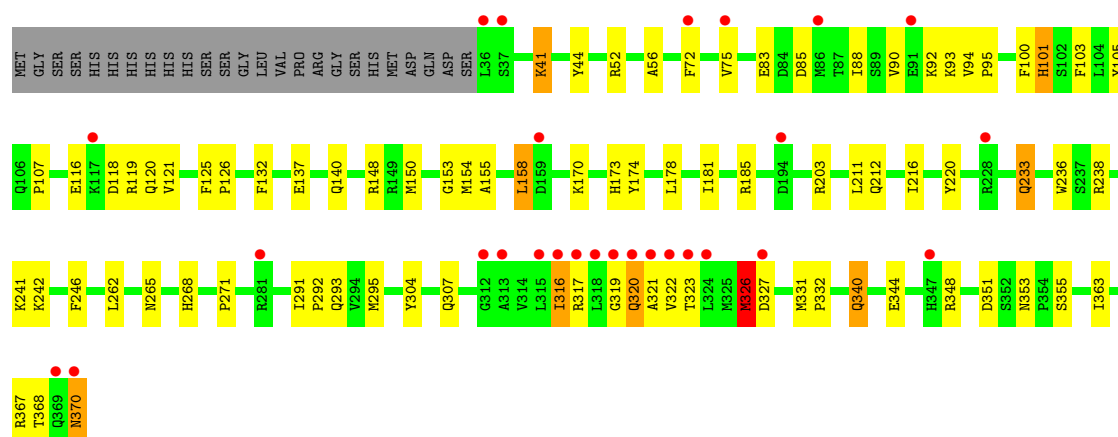
- Molecule 1: Squalene synthase



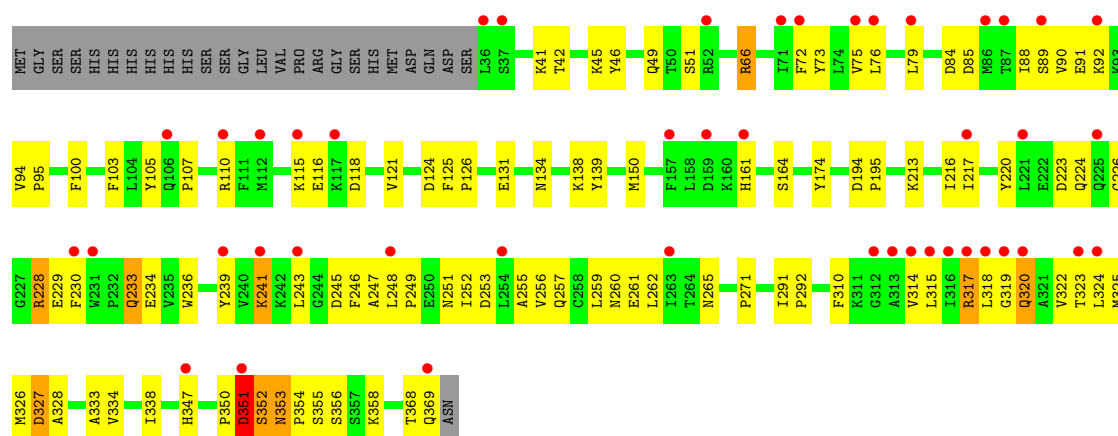
- Molecule 1: Squalene synthase

Chain D: 

- Molecule 1: Squalene synthase

Chain E: 

- Molecule 1: Squalene synthase

Chain F: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.33Å 153.62Å 92.11Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.86 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.20) 93.8 (24.86-2.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.225 0.199 , 0.227	Depositor DCC
$R_{free}$ test set	5697 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.8	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 114146 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E5S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/2751	0.59	0/3724
1	B	0.37	0/2732	0.57	1/3698 (0.0%)
1	C	0.36	0/2759	0.57	0/3735
1	D	0.34	0/2759	0.54	0/3735
1	E	0.33	0/2759	0.53	0/3735
1	F	0.32	0/2751	0.52	0/3724
All	All	0.35	0/16511	0.55	1/22351 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	LEU	CA-CB-CG	6.63	130.56	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2696	0	2676	50	0
1	B	2678	0	2651	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2704	0	2682	72	0
1	D	2704	0	2682	66	0
1	E	2704	0	2682	72	0
1	F	2696	0	2676	86	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
2	E	32	0	0	0	0
2	F	32	0	0	0	0
3	A	178	0	0	0	0
3	B	204	0	0	2	0
3	C	160	0	0	3	0
3	D	131	0	0	1	0
3	E	86	0	0	3	0
3	F	66	0	0	0	0
All	All	17199	0	16049	371	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (371) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:315:LEU:HG	1:C:316:ILE:H	1.20	1.04
1:E:319:GLY:HA3	1:E:323:THR:HG21	1.40	1.01
1:B:323:THR:O	1:B:325:MET:N	1.98	0.96
1:F:260:ASN:HD22	1:F:353:ASN:ND2	1.65	0.94
1:C:317:ARG:HG3	1:C:317:ARG:HH21	1.32	0.92
1:C:317:ARG:HB2	3:C:578:HOH:O	1.69	0.92
1:C:315:LEU:HG	1:C:316:ILE:N	1.86	0.91
1:F:233:GLN:HA	1:F:236:TRP:NE1	1.86	0.90
1:E:319:GLY:CA	1:E:323:THR:HG21	2.03	0.89
1:E:326:MET:HA	1:F:327:ASP:OD2	1.75	0.86
1:C:226:GLY:HA3	1:C:228:ARG:HH11	1.40	0.86
1:C:317:ARG:CG	1:C:317:ARG:HH21	1.89	0.85
1:A:320:GLN:HG3	1:A:340:GLN:HB3	1.58	0.83
1:F:228:ARG:HB2	1:F:228:ARG:NH1	1.94	0.82
1:F:318:LEU:HD12	1:F:318:LEU:H	1.44	0.82
1:E:320:GLN:HG2	1:E:321:ALA:H	1.46	0.80
1:A:320:GLN:O	1:A:323:THR:HG22	1.81	0.79
1:D:368:THR:HG21	1:E:41:LYS:HA	1.64	0.78
1:A:326:MET:HA	1:B:327:ASP:HB2	1.64	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:260:ASN:HD22	1:F:353:ASN:HD21	1.31	0.77
1:B:233:GLN:HA	1:B:236:TRP:NE1	1.99	0.77
1:A:319:GLY:CA	1:A:323:THR:HG21	2.15	0.76
1:B:120:GLN:NE2	1:B:120:GLN:H	1.82	0.76
1:A:323:THR:HG23	1:A:324:LEU:N	2.00	0.75
1:E:326:MET:HA	1:F:327:ASP:CG	2.07	0.75
1:A:319:GLY:HA2	1:A:323:THR:HG21	1.69	0.74
1:A:320:GLN:NE2	1:A:344:GLU:HG3	2.02	0.74
1:F:233:GLN:HA	1:F:236:TRP:CD1	2.23	0.74
1:B:322:VAL:HG12	1:B:340:GLN:NE2	2.03	0.73
1:C:226:GLY:HA3	1:C:228:ARG:NH1	2.03	0.72
1:E:150:MET:HG3	1:E:174:TYR:O	1.90	0.72
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.05	0.71
1:D:235:VAL:HA	1:D:238:ARG:HH21	1.53	0.71
1:E:105:TYR:O	1:E:107:PRO:HD3	1.91	0.70
1:E:90:VAL:O	1:E:94:VAL:HG23	1.91	0.70
1:D:327:ASP:CG	1:F:326:MET:HA	2.12	0.69
1:C:320:GLN:HG2	1:C:321:ALA:H	1.57	0.69
1:D:327:ASP:OD1	1:F:326:MET:HA	1.92	0.69
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.27	0.69
1:F:319:GLY:HA3	1:F:323:THR:HG21	1.74	0.69
1:A:357:SER:O	1:A:361:GLN:HG3	1.93	0.68
1:F:229:GLU:HB2	1:F:243:LEU:HD13	1.76	0.68
1:B:326:MET:HE3	1:C:291:ILE:HD11	1.76	0.67
1:C:314:VAL:HG12	1:C:315:LEU:H	1.60	0.67
1:D:94:VAL:HB	1:D:95:PRO:HD3	1.77	0.66
1:D:365:THR:O	1:D:369:GLN:HB3	1.95	0.66
1:B:118:ASP:C	1:B:120:GLN:HE21	1.99	0.66
1:A:323:THR:HG23	1:A:324:LEU:H	1.61	0.66
1:E:93:LYS:HD2	1:E:158:LEU:HD11	1.76	0.65
1:A:322:VAL:HG12	1:A:326:MET:SD	2.36	0.65
1:E:155:ALA:O	1:E:158:LEU:HB2	1.96	0.65
1:A:327:ASP:OD1	1:C:327:ASP:HB3	1.97	0.65
1:F:105:TYR:O	1:F:107:PRO:HD3	1.96	0.65
1:F:320:GLN:O	1:F:324:LEU:HG	1.98	0.64
1:A:218:ARG:NH1	1:A:219:ASP:OD1	2.31	0.64
1:A:320:GLN:HB2	1:A:340:GLN:OE1	1.98	0.64
1:A:248:LEU:HD23	1:A:250:GLU:OE1	1.98	0.63
1:C:315:LEU:HG	1:C:316:ILE:HG12	1.81	0.63
1:C:315:LEU:CG	1:C:316:ILE:N	2.58	0.63
1:D:368:THR:HG22	1:E:44:TYR:HB2	1.79	0.63
1:E:118:ASP:O	1:E:121:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:MET:HE2	1:A:333:ALA:HA	1.80	0.63
1:C:365:THR:O	1:C:369:GLN:HG3	1.98	0.63
1:C:320:GLN:HG2	1:C:321:ALA:N	2.14	0.62
1:A:245:ASP:HA	1:A:248:LEU:HD13	1.81	0.62
1:C:317:ARG:NH2	1:C:317:ARG:HG3	2.05	0.62
1:E:132:PHE:CZ	1:E:140:GLN:HB2	2.34	0.62
1:E:353:ASN:ND2	1:E:355:SER:H	1.98	0.62
1:F:89:SER:HB2	1:F:91:GLU:OE1	2.00	0.62
1:C:118:ASP:O	1:C:121:VAL:HG22	2.00	0.61
1:C:203:ARG:HD2	1:C:272:ASP:OD1	2.00	0.61
1:D:322:VAL:HG13	1:E:291:ILE:HG21	1.81	0.61
1:A:318:LEU:HB3	1:A:341:TYR:HE1	1.65	0.61
1:C:314:VAL:HG12	1:C:315:LEU:N	2.16	0.60
1:E:317:ARG:NH1	1:E:348:ARG:NH1	2.49	0.60
1:C:320:GLN:CG	1:C:321:ALA:H	2.13	0.60
1:D:100:PHE:HA	1:D:103:PHE:CD2	2.37	0.60
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.17	0.60
1:E:331:MET:HB3	1:E:332:PRO:HD3	1.84	0.60
1:F:236:TRP:CE2	1:F:243:LEU:HG	2.37	0.60
1:F:94:VAL:HB	1:F:95:PRO:HD3	1.83	0.60
1:B:353:ASN:ND2	1:B:355:SER:H	1.98	0.60
1:D:368:THR:HG21	1:E:41:LYS:HG3	1.84	0.60
1:B:323:THR:C	1:B:325:MET:H	1.99	0.59
1:F:322:VAL:O	1:F:325:MET:HB2	2.01	0.59
1:C:315:LEU:O	1:C:317:ARG:HD3	2.03	0.59
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.17	0.59
1:A:323:THR:CG2	1:A:324:LEU:N	2.65	0.59
1:B:117:LYS:O	1:B:120:GLN:NE2	2.35	0.59
1:D:308:GLN:NE2	1:D:311:LYS:HD2	2.18	0.59
1:D:299:THR:HA	1:D:316:ILE:HD11	1.84	0.59
1:C:94:VAL:HB	1:C:95:PRO:HD3	1.85	0.58
1:B:322:VAL:HA	1:C:295:MET:CE	2.33	0.58
1:F:228:ARG:HB2	1:F:228:ARG:CZ	2.32	0.58
1:C:348:ARG:O	1:C:350:PRO:HD3	2.03	0.58
1:B:110:ARG:NH2	3:B:534:HOH:O	2.37	0.58
1:B:252:ILE:HG23	1:B:253:ASP:N	2.18	0.58
1:F:118:ASP:O	1:F:121:VAL:HG22	2.04	0.57
1:D:370:ASN:H	1:D:370:ASN:ND2	2.02	0.57
1:D:363:ILE:O	1:D:367:ARG:HG2	2.02	0.57
1:A:323:THR:CG2	1:A:324:LEU:H	2.18	0.57
1:C:320:GLN:O	1:C:324:LEU:HG	2.03	0.57
1:B:190:SER:O	1:B:191:GLU:HB2	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:90:VAL:O	1:F:94:VAL:HG23	2.05	0.57
1:D:308:GLN:NE2	1:D:308:GLN:HA	2.20	0.57
1:B:323:THR:O	1:B:326:MET:N	2.37	0.56
1:A:233:GLN:HA	1:A:236:TRP:NE1	2.20	0.56
1:C:248:LEU:HB2	1:C:251:ASN:HD22	1.70	0.56
1:A:363:ILE:O	1:A:367:ARG:HG2	2.05	0.56
1:D:308:GLN:HE21	1:D:308:GLN:HA	1.69	0.56
1:F:260:ASN:ND2	1:F:353:ASN:HD21	2.03	0.56
1:C:353:ASN:ND2	1:C:355:SER:H	2.02	0.56
1:D:150:MET:HG3	1:D:174:TYR:O	2.03	0.56
1:B:150:MET:HG3	1:B:174:TYR:O	2.06	0.56
1:D:353:ASN:ND2	1:D:355:SER:H	2.04	0.56
1:D:71:ILE:O	1:D:75:VAL:HG13	2.06	0.56
1:E:212:GLN:HE21	1:E:216:ILE:HG13	1.70	0.56
1:C:318:LEU:O	1:C:318:LEU:HD23	2.06	0.56
1:B:252:ILE:HD11	1:B:307:GLN:HB3	1.88	0.55
1:D:370:ASN:HD22	1:D:370:ASN:H	1.52	0.55
1:D:319:GLY:HA3	1:D:323:THR:HG21	1.88	0.55
1:E:125:PHE:N	1:E:126:PRO:CD	2.69	0.55
1:C:100:PHE:HA	1:C:103:PHE:CD2	2.42	0.55
1:A:36:LEU:N	1:A:36:LEU:HD12	2.22	0.55
1:F:220:TYR:OH	1:F:246:PHE:HB2	2.06	0.55
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.89	0.55
1:C:195:PRO:O	1:C:199:GLU:HG3	2.07	0.55
1:B:325:MET:O	1:C:327:ASP:HB2	2.07	0.54
1:A:150:MET:HG3	1:A:174:TYR:O	2.07	0.54
1:A:326:MET:CE	1:A:333:ALA:HA	2.38	0.54
1:A:245:ASP:O	1:A:248:LEU:HB2	2.08	0.54
1:A:326:MET:HA	1:B:327:ASP:CB	2.33	0.54
1:D:348:ARG:O	1:D:350:PRO:HD3	2.08	0.54
1:A:41:LYS:HA	1:C:368:THR:HG21	1.89	0.54
1:C:105:TYR:O	1:C:107:PRO:HD3	2.07	0.54
1:D:327:ASP:OD2	1:D:328:ALA:N	2.40	0.54
1:F:325:MET:CE	1:F:325:MET:HA	2.38	0.54
1:A:353:ASN:ND2	1:A:355:SER:H	2.06	0.53
1:B:120:GLN:CD	1:B:120:GLN:H	2.09	0.53
1:E:320:GLN:CG	1:E:321:ALA:H	2.16	0.53
1:F:262:LEU:O	1:F:265:ASN:HB3	2.08	0.53
1:D:220:TYR:OH	1:D:246:PHE:HB2	2.08	0.53
1:F:45:LYS:HG2	1:F:49:GLN:HE21	1.74	0.53
1:D:163:THR:HA	1:D:233:GLN:HB3	1.91	0.53
1:D:299:THR:HA	1:D:316:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:150:MET:HG3	1:F:174:TYR:O	2.09	0.53
1:F:85:ASP:OD2	1:F:88:ILE:HG13	2.09	0.53
1:C:248:LEU:HB3	1:C:250:GLU:OE1	2.10	0.52
1:F:255:ALA:HB1	1:F:310:PHE:CE2	2.44	0.52
1:F:239:TYR:HE2	1:F:261:GLU:OE1	1.93	0.52
1:F:350:PRO:C	1:F:352:SER:H	2.13	0.52
1:F:247:ALA:O	1:F:249:PRO:HD3	2.10	0.52
1:C:318:LEU:HD23	1:C:324:LEU:HD21	1.91	0.52
1:D:326:MET:HE2	1:D:333:ALA:HA	1.92	0.52
1:B:322:VAL:HA	1:C:295:MET:HE3	1.91	0.52
1:D:327:ASP:OD2	1:F:325:MET:O	2.28	0.52
1:D:153:GLY:HA3	1:D:174:TYR:CG	2.45	0.51
1:E:56:ALA:HB3	3:E:520:HOH:O	2.10	0.51
1:F:326:MET:HE2	1:F:333:ALA:HA	1.91	0.51
1:E:344:GLU:O	1:E:348:ARG:HD3	2.10	0.51
1:D:218:ARG:HD2	1:D:219:ASP:OD1	2.11	0.51
1:F:115:LYS:NZ	1:F:115:LYS:HB3	2.24	0.51
1:D:370:ASN:HD22	1:D:370:ASN:N	2.08	0.51
1:D:45:LYS:O	1:D:49:GLN:HG3	2.11	0.51
1:E:153:GLY:HA3	1:E:174:TYR:CG	2.45	0.51
1:F:260:ASN:ND2	1:F:353:ASN:ND2	2.48	0.51
1:B:218:ARG:HD2	1:B:219:ASP:OD1	2.11	0.51
1:B:369:GLN:HB2	3:B:679:HOH:O	2.10	0.51
1:C:51:SER:HB2	1:C:73:TYR:CZ	2.46	0.51
1:C:316:ILE:C	1:C:318:LEU:H	2.14	0.51
1:D:125:PHE:N	1:D:126:PRO:CD	2.73	0.50
1:F:320:GLN:O	1:F:323:THR:HG22	2.12	0.50
1:B:343:GLU:OE1	1:B:367:ARG:NH2	2.43	0.50
1:E:236:TRP:CZ3	1:E:242:LYS:HA	2.46	0.50
1:F:138:LYS:HE3	1:F:139:TYR:CZ	2.47	0.50
1:E:323:THR:HB	1:E:340:GLN:NE2	2.26	0.50
1:F:89:SER:OG	1:F:92:LYS:HB2	2.12	0.50
1:C:326:MET:HE2	1:C:333:ALA:HA	1.94	0.50
1:E:295:MET:CE	1:E:295:MET:HA	2.42	0.50
1:F:228:ARG:HB2	1:F:228:ARG:HH11	1.71	0.50
1:E:323:THR:HA	1:E:326:MET:CG	2.42	0.50
1:F:79:LEU:HB2	1:F:100:PHE:CE2	2.46	0.50
1:F:291:ILE:HB	1:F:292:PRO:HD3	1.94	0.50
1:E:322:VAL:HB	1:E:340:GLN:OE1	2.12	0.49
1:F:236:TRP:HZ3	1:F:241:LYS:C	2.16	0.49
1:A:170:LYS:HE2	1:A:174:TYR:OH	2.12	0.49
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:75:VAL:HG23	1:F:76:LEU:N	2.27	0.49
1:E:320:GLN:HG2	1:E:321:ALA:N	2.21	0.49
1:D:242:LYS:HB2	1:D:245:ASP:OD2	2.13	0.49
1:E:92:LYS:O	1:E:95:PRO:HD2	2.11	0.49
1:A:248:LEU:HB2	1:A:251:ASN:HD22	1.78	0.49
1:A:291:ILE:HG21	1:C:322:VAL:HG13	1.94	0.49
1:C:317:ARG:O	1:C:319:GLY:N	2.45	0.49
1:D:252:ILE:O	1:D:256:VAL:HG23	2.12	0.49
1:E:233:GLN:HA	1:E:236:TRP:CD1	2.48	0.49
1:F:115:LYS:HB3	1:F:115:LYS:HZ2	1.77	0.49
1:C:170:LYS:HA	3:C:585:HOH:O	2.11	0.49
1:D:259:LEU:HB2	1:D:310:PHE:HZ	1.76	0.49
1:C:190:SER:O	1:C:191:GLU:HB2	2.13	0.49
1:E:233:GLN:HA	1:E:236:TRP:CE2	2.48	0.49
1:D:319:GLY:C	1:D:323:THR:HB	2.33	0.49
1:E:170:LYS:O	1:E:173:HIS:HB3	2.13	0.48
1:B:353:ASN:HD21	1:B:355:SER:HB2	1.77	0.48
1:C:250:GLU:CD	1:C:250:GLU:H	2.17	0.48
1:E:320:GLN:HB3	1:E:340:GLN:OE1	2.14	0.48
1:B:322:VAL:HA	1:C:295:MET:HE1	1.96	0.48
1:E:307:GLN:HG3	3:E:513:HOH:O	2.13	0.48
1:B:233:GLN:HA	1:B:236:TRP:CD1	2.49	0.48
1:D:291:ILE:HB	1:D:292:PRO:HD3	1.95	0.48
1:A:326:MET:CA	1:B:327:ASP:HB2	2.40	0.47
1:C:364:SER:O	1:C:368:THR:HG23	2.14	0.47
1:A:114:SER:O	1:A:119:ARG:HD3	2.14	0.47
1:F:125:PHE:N	1:F:126:PRO:CD	2.77	0.47
1:B:125:PHE:N	1:B:126:PRO:CD	2.77	0.47
1:D:233:GLN:HA	1:D:236:TRP:CE2	2.50	0.47
1:C:150:MET:O	1:C:154:MET:HG3	2.14	0.47
1:D:67:ASN:O	1:D:71:ILE:HG12	2.15	0.47
1:C:320:GLN:CG	1:C:321:ALA:N	2.77	0.47
1:B:323:THR:HG22	1:B:340:GLN:OE1	2.14	0.47
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.96	0.47
1:E:326:MET:HE3	1:F:291:ILE:HD11	1.97	0.47
1:E:304:TYR:O	1:E:348:ARG:NH2	2.47	0.47
1:E:72:PHE:O	1:E:75:VAL:HG22	2.15	0.47
1:D:316:ILE:O	1:D:316:ILE:HG22	2.16	0.46
1:F:325:MET:HA	1:F:325:MET:HE2	1.97	0.46
1:E:319:GLY:CA	1:E:323:THR:CG2	2.87	0.46
1:C:193:GLU:HB3	1:C:197:VAL:HG21	1.98	0.46
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ARG:O	1:A:123:GLU:HG3	2.15	0.46
1:C:228:ARG:H	1:C:228:ARG:HD3	1.80	0.46
1:E:291:ILE:HB	1:E:292:PRO:HD3	1.98	0.46
1:E:92:LYS:C	1:E:95:PRO:HD2	2.35	0.46
1:D:185:ARG:HD2	3:D:512:HOH:O	2.16	0.46
1:D:338:ILE:O	1:D:342:MET:HG2	2.16	0.46
1:E:116:GLU:O	1:E:119:ARG:HG3	2.15	0.46
1:E:85:ASP:HB3	1:E:88:ILE:HD12	1.98	0.46
1:A:125:PHE:N	1:A:126:PRO:CD	2.79	0.45
1:C:250:GLU:N	1:C:250:GLU:OE2	2.49	0.45
1:D:119:ARG:O	1:D:123:GLU:HG3	2.15	0.45
1:D:246:PHE:CD1	1:D:255:ALA:HA	2.51	0.45
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.52	0.45
1:E:368:THR:OG1	1:F:41:LYS:HA	2.16	0.45
1:F:72:PHE:CZ	1:F:76:LEU:HD11	2.52	0.45
1:E:94:VAL:N	1:E:95:PRO:CD	2.80	0.45
1:F:51:SER:HB2	1:F:73:TYR:CZ	2.51	0.45
1:D:325:MET:O	1:E:327:ASP:HB2	2.17	0.45
1:B:306:ASN:OD1	1:B:308:GLN:HB2	2.17	0.44
1:C:87:THR:OG1	1:C:115:LYS:HG2	2.17	0.44
1:F:245:ASP:O	1:F:248:LEU:HB2	2.17	0.44
1:F:246:PHE:CD1	1:F:255:ALA:HA	2.52	0.44
1:C:157:PHE:CE2	1:C:160:LYS:HE3	2.52	0.44
1:E:370:ASN:HB3	1:F:66:ARG:CD	2.47	0.44
1:F:334:VAL:O	1:F:338:ILE:HG13	2.18	0.44
1:B:153:GLY:HA3	1:B:174:TYR:CG	2.52	0.44
1:D:105:TYR:O	1:D:107:PRO:HD3	2.18	0.44
1:D:308:GLN:HE22	1:D:311:LYS:HD2	1.83	0.44
1:E:268:HIS:O	1:E:271:PRO:HD2	2.17	0.44
1:B:262:LEU:O	1:B:265:ASN:HB3	2.18	0.44
1:D:153:GLY:HA3	1:D:174:TYR:CD1	2.53	0.44
1:F:131:GLU:HA	1:F:134:ASN:HD22	1.83	0.44
1:F:248:LEU:HB2	1:F:251:ASN:HD22	1.82	0.44
1:F:318:LEU:H	1:F:318:LEU:CD1	2.21	0.44
1:A:52:ARG:CG	1:A:52:ARG:HH11	2.29	0.43
1:E:93:LYS:CD	1:E:158:LEU:HD11	2.47	0.43
1:C:233:GLN:HA	1:C:236:TRP:CD1	2.53	0.43
1:D:41:LYS:HA	1:F:368:THR:HG21	1.99	0.43
1:F:194:ASP:OD1	1:F:195:PRO:HD2	2.18	0.43
1:A:289:CYS:O	1:A:293:GLN:HG2	2.18	0.43
1:D:320:GLN:O	1:D:321:ALA:C	2.56	0.43
1:B:291:ILE:HB	1:B:292:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:317:ARG:HD2	1:C:317:ARG:HA	1.89	0.43
1:A:327:ASP:HB3	1:C:326:MET:HA	2.00	0.43
1:D:190:SER:O	1:D:191:GLU:HB2	2.18	0.43
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.32	0.43
1:F:124:ASP:O	1:F:124:ASP:CG	2.57	0.43
1:F:85:ASP:HA	1:F:116:GLU:OE2	2.17	0.43
1:B:246:PHE:CD1	1:B:255:ALA:HA	2.53	0.43
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.87	0.43
1:B:353:ASN:ND2	1:B:355:SER:HB2	2.34	0.43
1:C:67:ASN:O	1:C:71:ILE:HG12	2.18	0.43
1:F:353:ASN:HA	1:F:354:PRO:HD3	1.79	0.43
1:F:92:LYS:C	1:F:95:PRO:HD2	2.39	0.43
1:A:316:ILE:N	1:A:316:ILE:HD12	2.33	0.43
1:E:181:ILE:O	1:E:185:ARG:HG3	2.19	0.43
1:F:239:TYR:HE1	1:F:257:GLN:HE21	1.67	0.43
1:C:297:ILE:CD1	1:C:338:ILE:HG12	2.49	0.43
1:E:137:GLU:HA	1:E:140:GLN:HG2	2.00	0.43
1:E:211:LEU:HG	1:E:293:GLN:HE22	1.83	0.43
1:E:83:GLU:HB2	1:E:154:MET:HE2	2.00	0.43
1:A:252:ILE:HG23	1:A:253:ASP:N	2.33	0.42
1:B:263:ILE:O	1:B:267:LEU:HG	2.18	0.42
1:F:213:LYS:O	1:F:217:ILE:HG13	2.19	0.42
1:A:233:GLN:HA	1:A:236:TRP:CD1	2.54	0.42
1:C:114:SER:C	1:C:115:LYS:HD2	2.39	0.42
1:D:229:GLU:HG2	1:D:243:LEU:HD23	2.02	0.42
1:E:320:GLN:O	1:E:323:THR:HG22	2.19	0.42
1:F:317:ARG:HG3	1:F:318:LEU:O	2.20	0.42
1:B:326:MET:HA	1:C:327:ASP:HB2	2.02	0.42
1:E:101:HIS:ND1	1:E:148:ARG:HB2	2.34	0.42
1:D:343:GLU:OE1	1:D:367:ARG:NH2	2.52	0.42
1:F:355:SER:O	1:F:358:LYS:N	2.52	0.42
1:B:326:MET:HE3	1:C:291:ILE:CD1	2.44	0.42
1:F:271:PRO:HA	1:F:369:GLN:HE22	1.84	0.42
1:B:71:ILE:HG21	1:B:132:PHE:HA	2.02	0.42
1:B:323:THR:O	1:B:326:MET:HG3	2.19	0.42
1:C:331:MET:HB3	1:C:332:PRO:HD3	2.02	0.42
1:E:320:GLN:CG	1:E:321:ALA:N	2.81	0.42
1:F:256:VAL:O	1:F:259:LEU:HB3	2.19	0.42
1:A:233:GLN:HE21	1:A:233:GLN:HB3	1.62	0.42
1:B:113:GLU:O	1:B:115:LYS:HD2	2.20	0.42
1:B:193:GLU:OE1	1:B:193:GLU:HA	2.19	0.42
1:E:295:MET:HE2	1:E:295:MET:HA	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:42:THR:HG22	1:F:46:TYR:CE2	2.55	0.42
1:B:220:TYR:HB2	1:B:231:TRP:CZ2	2.54	0.42
1:C:241:LYS:HE3	1:C:241:LYS:HB3	1.85	0.42
1:D:344:GLU:HG2	1:D:348:ARG:HH12	1.85	0.42
1:D:356:SER:O	1:D:360:ARG:HG3	2.18	0.42
1:E:317:ARG:HB2	3:E:507:HOH:O	2.19	0.42
1:F:92:LYS:O	1:F:95:PRO:HD2	2.20	0.42
1:D:331:MET:HB3	1:D:332:PRO:HD3	2.02	0.42
1:D:320:GLN:HB3	1:D:340:GLN:OE1	2.19	0.42
1:E:353:ASN:HD21	1:E:355:SER:HB2	1.85	0.42
1:F:220:TYR:CZ	1:F:246:PHE:HB2	2.54	0.42
1:F:223:ASP:O	1:F:228:ARG:O	2.37	0.42
1:F:355:SER:O	1:F:356:SER:C	2.58	0.42
1:F:216:ILE:HG23	1:F:230:PHE:HB2	2.02	0.41
1:F:241:LYS:NZ	1:F:241:LYS:HB2	2.35	0.41
1:C:252:ILE:HG23	1:C:253:ASP:N	2.34	0.41
1:D:262:LEU:O	1:D:265:ASN:HB3	2.21	0.41
1:F:224:GLN:C	1:F:226:GLY:H	2.23	0.41
1:F:252:ILE:HG23	1:F:253:ASP:N	2.36	0.41
1:F:318:LEU:N	1:F:318:LEU:HD12	2.22	0.41
1:E:363:ILE:O	1:E:367:ARG:HG3	2.20	0.41
1:F:164:SER:HB3	1:F:234:GLU:OE1	2.20	0.41
1:A:353:ASN:HA	1:A:354:PRO:HD3	1.83	0.41
1:B:118:ASP:O	1:B:121:VAL:HG22	2.21	0.41
1:B:233:GLN:HE21	1:B:233:GLN:HB3	1.57	0.41
1:B:252:ILE:CG2	1:B:253:ASP:N	2.84	0.41
1:E:326:MET:N	1:F:327:ASP:HB2	2.35	0.41
1:B:150:MET:O	1:B:154:MET:HG3	2.19	0.41
1:B:334:VAL:O	1:B:338:ILE:HG13	2.21	0.41
1:B:356:SER:O	1:B:360:ARG:HG3	2.20	0.41
1:E:370:ASN:HB3	1:F:66:ARG:HD3	2.03	0.41
1:A:120:GLN:HG2	1:A:121:VAL:N	2.36	0.41
1:A:291:ILE:HB	1:A:292:PRO:HD3	2.02	0.41
1:A:304:TYR:CD2	1:A:345:ILE:HG23	2.56	0.41
1:B:77:ARG:HD3	1:B:77:ARG:HA	1.90	0.41
1:E:150:MET:HG2	1:E:154:MET:SD	2.61	0.41
1:E:233:GLN:HB3	1:E:233:GLN:HE21	1.71	0.41
1:E:94:VAL:HB	1:E:95:PRO:HD3	2.02	0.41
1:A:322:VAL:CG1	1:A:326:MET:SD	3.07	0.41
1:D:263:ILE:O	1:D:267:LEU:HG	2.21	0.41
1:D:334:VAL:O	1:D:338:ILE:HG13	2.20	0.41
1:C:59:GLN:HE21	1:C:59:GLN:HB2	1.75	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:259:LEU:HD21	1:D:303:CYS:O	2.20	0.40
1:B:233:GLN:HA	1:B:236:TRP:CE2	2.55	0.40
1:F:351:ASP:OD1	1:F:351:ASP:N	2.45	0.40
1:A:190:SER:O	1:A:191:GLU:HB2	2.20	0.40
1:C:198:GLY:HA3	3:C:592:HOH:O	2.21	0.40
1:C:236:TRP:CZ3	1:C:242:LYS:HA	2.57	0.40
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.56	0.40
1:C:356:SER:O	1:C:360:ARG:HG3	2.20	0.40
1:B:353:ASN:HD22	1:B:355:SER:H	1.66	0.40
1:C:125:PHE:N	1:C:126:PRO:CD	2.85	0.40
1:C:248:LEU:HB2	1:C:251:ASN:ND2	2.34	0.40
1:D:118:ASP:O	1:D:121:VAL:HG22	2.22	0.40
1:E:220:TYR:CZ	1:E:246:PHE:HB2	2.56	0.40
1:E:262:LEU:O	1:E:265:ASN:HB3	2.21	0.40
1:F:72:PHE:CE1	1:F:76:LEU:HD11	2.56	0.40
1:E:178:LEU:HD23	1:E:181:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	318 (96%)	13 (4%)	1 (0%)	50	53
1	B	328/360 (91%)	314 (96%)	12 (4%)	2 (1%)	33	32
1	C	333/360 (92%)	320 (96%)	10 (3%)	3 (1%)	25	21
1	D	333/360 (92%)	315 (95%)	14 (4%)	4 (1%)	19	14
1	E	333/360 (92%)	315 (95%)	15 (4%)	3 (1%)	25	21
1	F	332/360 (92%)	305 (92%)	24 (7%)	3 (1%)	25	21
All	All	1991/2160 (92%)	1887 (95%)	88 (4%)	16 (1%)	27	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LEU
1	B	324	LEU
1	C	316	ILE
1	C	318	LEU
1	D	320	GLN
1	E	316	ILE
1	F	328	ALA
1	D	318	LEU
1	E	320	GLN
1	D	321	ALA
1	C	63	GLY
1	D	63	GLY
1	E	326	MET
1	F	66	ARG
1	F	351	ASP
1	B	63	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/320 (93%)	285 (96%)	12 (4%)	42	51
1	B	296/320 (92%)	286 (97%)	10 (3%)	49	59
1	C	298/320 (93%)	290 (97%)	8 (3%)	57	68
1	D	298/320 (93%)	287 (96%)	11 (4%)	45	54
1	E	298/320 (93%)	284 (95%)	14 (5%)	36	42
1	F	297/320 (93%)	282 (95%)	15 (5%)	33	38
All	All	1784/1920 (93%)	1714 (96%)	70 (4%)	43	52

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	52	ARG
1	A	84	ASP
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	119	ARG
1	A	167	GLU
1	A	203	ARG
1	A	218	ARG
1	A	233	GLN
1	A	320	GLN
1	A	324	LEU
1	A	351	ASP
1	B	77	ARG
1	B	110	ARG
1	B	115	LYS
1	B	120	GLN
1	B	233	GLN
1	B	238	ARG
1	B	315	LEU
1	B	322	VAL
1	B	323	THR
1	B	326	MET
1	C	110	ARG
1	C	203	ARG
1	C	228	ARG
1	C	233	GLN
1	C	242	LYS
1	C	315	LEU
1	C	317	ARG
1	C	368	THR
1	D	36	LEU
1	D	77	ARG
1	D	91	GLU
1	D	203	ARG
1	D	233	GLN
1	D	241	LYS
1	D	315	LEU
1	D	317	ARG
1	D	347	HIS
1	D	369	GLN
1	D	370	ASN
1	E	41	LYS
1	E	52	ARG
1	E	101	HIS
1	E	120	GLN
1	E	158	LEU

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Mol	Chain	Res	Type
1	E	203	ARG
1	E	233	GLN
1	E	238	ARG
1	E	241	LYS
1	E	316	ILE
1	E	326	MET
1	E	340	GLN
1	E	351	ASP
1	E	370	ASN
1	F	84	ASP
1	F	110	ARG
1	F	161	HIS
1	F	228	ARG
1	F	233	GLN
1	F	241	LYS
1	F	314	VAL
1	F	315	LEU
1	F	317	ARG
1	F	320	GLN
1	F	327	ASP
1	F	347	HIS
1	F	351	ASP
1	F	352	SER
1	F	353	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	233	GLN
1	A	251	ASN
1	A	257	GLN
1	A	308	GLN
1	A	320	GLN
1	A	361	GLN
1	B	120	GLN
1	B	225	GLN
1	B	233	GLN
1	B	251	ASN
1	B	257	GLN
1	B	308	GLN
1	B	340	GLN

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Mol	Chain	Res	Type
1	C	49	GLN
1	C	225	GLN
1	C	251	ASN
1	C	257	GLN
1	D	225	GLN
1	D	233	GLN
1	D	257	GLN
1	D	308	GLN
1	D	353	ASN
1	D	370	ASN
1	E	49	GLN
1	E	212	GLN
1	E	225	GLN
1	E	233	GLN
1	E	257	GLN
1	E	293	GLN
1	E	353	ASN
1	F	134	ASN
1	F	161	HIS
1	F	225	GLN
1	F	233	GLN
1	F	251	ASN
1	F	257	GLN
1	F	308	GLN
1	F	353	ASN
1	F	369	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	E5S	A	901	-	36,36,36	2.57	4 (11%)	52,52,52	1.58	5 (9%)
2	E5S	B	401	-	36,36,36	2.54	4 (11%)	52,52,52	1.59	3 (5%)
2	E5S	C	401	-	36,36,36	2.57	4 (11%)	52,52,52	1.60	5 (9%)
2	E5S	D	401	-	36,36,36	2.59	4 (11%)	52,52,52	1.65	6 (11%)
2	E5S	E	401	-	36,36,36	2.59	4 (11%)	52,52,52	1.56	4 (7%)
2	E5S	F	401	-	36,36,36	2.60	4 (11%)	52,52,52	1.58	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E5S	A	901	-	-	0/16/49/49	0/3/5/5
2	E5S	B	401	-	-	0/16/49/49	0/3/5/5
2	E5S	C	401	-	-	0/16/49/49	0/3/5/5
2	E5S	D	401	-	-	0/16/49/49	0/3/5/5
2	E5S	E	401	-	-	0/16/49/49	0/3/5/5
2	E5S	F	401	-	-	0/16/49/49	0/3/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	E5S	CAQ-CAZ	-14.34	1.39	1.51
2	E	401	E5S	CAQ-CAZ	-14.33	1.39	1.51
2	D	401	E5S	CAQ-CAZ	-14.32	1.39	1.51
2	A	901	E5S	CAQ-CAZ	-14.24	1.39	1.51
2	C	401	E5S	CAQ-CAZ	-14.11	1.39	1.51
2	B	401	E5S	CAQ-CAZ	-14.07	1.39	1.51
2	A	901	E5S	CAQ-CAW	-3.48	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	E5S	CAQ-CAW	-3.48	1.39	1.52
2	D	401	E5S	CAQ-CAW	-3.48	1.39	1.52
2	F	401	E5S	CAQ-CAW	-3.47	1.39	1.52
2	C	401	E5S	CAQ-CAW	-3.45	1.39	1.52
2	B	401	E5S	CAQ-CAW	-3.41	1.39	1.52
2	C	401	E5S	CAD-CAE	2.82	1.23	1.19
2	F	401	E5S	CAD-CAE	2.56	1.22	1.19
2	E	401	E5S	CAD-CAE	2.55	1.22	1.19
2	D	401	E5S	CAD-CAE	2.43	1.22	1.19
2	B	401	E5S	CAD-CAE	2.42	1.22	1.19
2	A	901	E5S	CAD-CAE	2.38	1.22	1.19
2	E	401	E5S	CAY-NBE	-2.18	1.33	1.37
2	F	401	E5S	CAY-NBE	-2.14	1.33	1.37
2	C	401	E5S	CAY-NBE	-2.13	1.33	1.37
2	A	901	E5S	CAY-NBE	-2.12	1.33	1.37
2	D	401	E5S	CAY-NBE	-2.05	1.33	1.37
2	B	401	E5S	CAY-NBE	-2.02	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	E5S	CAR-CBA-CBC	-7.76	98.52	104.37
2	C	401	E5S	CAR-CBA-CBC	-7.17	98.96	104.37
2	B	401	E5S	CAR-CBA-CBC	-7.16	98.97	104.37
2	F	401	E5S	CAR-CBA-CBC	-7.16	98.97	104.37
2	E	401	E5S	CAR-CBA-CBC	-7.08	99.03	104.37
2	A	901	E5S	CAR-CBA-CBC	-6.78	99.25	104.37
2	C	401	E5S	CAY-NAU-CAZ	5.47	122.20	118.52
2	B	401	E5S	CAY-NAU-CAZ	5.11	121.96	118.52
2	D	401	E5S	CAY-NAU-CAZ	5.03	121.90	118.52
2	A	901	E5S	CAY-NAU-CAZ	4.93	121.84	118.52
2	E	401	E5S	CAY-NAU-CAZ	4.92	121.83	118.52
2	F	401	E5S	CAY-NAU-CAZ	4.81	121.76	118.52
2	F	401	E5S	CAN-CBB-CBF	-2.79	108.04	109.51
2	A	901	E5S	NAU-CAY-NBE	2.73	119.91	116.64
2	D	401	E5S	CAN-CBB-CBF	-2.50	108.19	109.51
2	C	401	E5S	CAL-CAY-NAU	-2.30	119.96	123.56
2	C	401	E5S	CAN-CBB-CBF	-2.22	108.34	109.51
2	E	401	E5S	CAM-CBB-CBF	-2.12	108.39	109.51
2	D	401	E5S	CAL-CAY-NAU	-2.09	120.29	123.56
2	E	401	E5S	CAL-CAY-NAU	-2.09	120.29	123.56
2	C	401	E5S	CAR-NBE-CAS	-2.09	108.32	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	E5S	CAT-CBF-CAE	-2.07	108.21	112.50
2	A	901	E5S	CAN-CBB-CBF	-2.05	108.43	109.51
2	B	401	E5S	CAM-CBB-CBF	-2.05	108.43	109.51
2	F	401	E5S	CAL-CAY-NAU	-2.04	120.37	123.56
2	A	901	E5S	CAL-CAY-NAU	-2.04	120.38	123.56
2	D	401	E5S	CAR-NBE-CAS	-2.01	108.50	112.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/360 (92%)	-0.20	14 (4%)	35 35	16, 27, 57, 101	0
1	B	332/360 (92%)	-0.06	14 (4%)	35 35	16, 30, 68, 95	0
1	C	335/360 (93%)	0.06	18 (5%)	25 25	20, 32, 64, 107	0
1	D	335/360 (93%)	0.18	26 (7%)	13 12	22, 38, 79, 112	0
1	E	335/360 (93%)	0.38	27 (8%)	12 11	29, 48, 82, 113	0
1	F	334/360 (92%)	0.73	45 (13%)	4 4	25, 59, 91, 112	0
All	All	2005/2160 (92%)	0.18	144 (7%)	15 15	16, 39, 84, 113	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	LEU	8.6
1	C	318	LEU	8.4
1	D	36	LEU	8.2
1	F	318	LEU	8.1
1	A	318	LEU	7.9
1	C	313	ALA	7.3
1	F	315	LEU	6.8
1	C	319	GLY	6.4
1	F	320	GLN	6.4
1	F	324	LEU	6.3
1	D	317	ARG	6.2
1	C	321	ALA	6.0
1	F	36	LEU	5.8
1	A	315	LEU	5.8
1	C	316	ILE	5.7
1	D	313	ALA	5.6
1	F	317	ARG	5.6
1	D	315	LEU	5.5
1	E	317	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	324	LEU	5.4
1	E	320	GLN	5.3
1	C	315	LEU	5.3
1	E	318	LEU	5.3
1	E	313	ALA	5.3
1	F	313	ALA	5.3
1	F	319	GLY	5.2
1	D	319	GLY	5.1
1	A	319	GLY	5.1
1	E	36	LEU	5.1
1	F	316	ILE	5.1
1	C	320	GLN	5.0
1	D	323	THR	5.0
1	B	315	LEU	4.9
1	F	323	THR	4.9
1	D	312	GLY	4.9
1	C	36	LEU	4.9
1	D	316	ILE	4.7
1	B	313	ALA	4.7
1	A	320	GLN	4.6
1	F	241	LYS	4.5
1	B	312	GLY	4.4
1	F	159	ASP	4.4
1	E	323	THR	4.3
1	D	37	SER	4.1
1	E	319	GLY	4.1
1	D	321	ALA	3.9
1	B	370	ASN	3.9
1	A	36	LEU	3.8
1	C	312	GLY	3.8
1	B	316	ILE	3.8
1	E	321	ALA	3.7
1	A	317	ARG	3.7
1	E	370	ASN	3.6
1	F	312	GLY	3.6
1	F	351	ASP	3.6
1	B	323	THR	3.6
1	D	320	GLN	3.5
1	F	225	GLN	3.5
1	E	91	GLU	3.4
1	E	86	MET	3.3
1	A	313	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	3.1
1	F	89	SER	3.1
1	F	87	THR	3.1
1	D	159	ASP	3.1
1	E	315	LEU	3.1
1	E	37	SER	3.1
1	F	92	LYS	3.1
1	F	230	PHE	3.1
1	C	317	ARG	3.1
1	A	323	THR	3.1
1	F	217	ILE	3.0
1	D	347	HIS	3.0
1	F	231	TRP	2.9
1	B	324	LEU	2.9
1	C	314	VAL	2.9
1	D	228	ARG	2.9
1	D	115	LYS	2.8
1	F	115	LYS	2.8
1	F	75	VAL	2.8
1	F	248	LEU	2.8
1	F	239	TYR	2.8
1	E	159	ASP	2.7
1	E	281	ARG	2.7
1	F	110	ARG	2.7
1	E	322	VAL	2.7
1	C	323	THR	2.6
1	D	248	LEU	2.6
1	F	221	LEU	2.6
1	C	228	ARG	2.6
1	F	37	SER	2.6
1	A	322	VAL	2.6
1	E	117	LYS	2.6
1	C	248	LEU	2.5
1	E	75	VAL	2.5
1	D	225	GLN	2.5
1	E	194	ASP	2.5
1	F	76	LEU	2.5
1	F	254	LEU	2.5
1	E	228	ARG	2.5
1	D	314	VAL	2.4
1	D	324	LEU	2.4
1	A	316	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	161	HIS	2.4
1	B	259	LEU	2.4
1	F	243	LEU	2.4
1	F	369	GLN	2.4
1	C	370	ASN	2.3
1	E	324	LEU	2.3
1	B	325	MET	2.3
1	E	312	GLY	2.3
1	F	157	PHE	2.3
1	C	52	ARG	2.3
1	F	347	HIS	2.3
1	F	106	GLN	2.3
1	B	241	LYS	2.2
1	F	71	ILE	2.2
1	B	231	TRP	2.2
1	B	159	ASP	2.2
1	D	52	ARG	2.2
1	B	347	HIS	2.2
1	D	91	GLU	2.2
1	E	327	ASP	2.2
1	E	316	ILE	2.1
1	F	86	MET	2.1
1	F	314	VAL	2.1
1	F	52	ARG	2.1
1	C	159	ASP	2.1
1	B	248	LEU	2.1
1	D	325	MET	2.1
1	F	263	ILE	2.1
1	D	241	LYS	2.1
1	E	72	PHE	2.1
1	F	72	PHE	2.1
1	A	76	LEU	2.1
1	D	310	PHE	2.1
1	E	347	HIS	2.1
1	F	117	LYS	2.1
1	C	324	LEU	2.0
1	F	79	LEU	2.0
1	A	314	VAL	2.0
1	E	369	GLN	2.0
1	F	112	MET	2.0
1	D	236	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	E5S	F	401	32/32	0.19	0.81	44,53,63,63	0
2	E5S	C	401	32/32	0.16	0.74	25,37,48,48	0
2	E5S	A	901	32/32	0.14	0.56	18,36,44,45	0
2	E5S	E	401	32/32	0.16	0.31	38,42,51,51	0
2	E5S	D	401	32/32	0.12	0.17	25,37,50,51	0
2	E5S	B	401	32/32	0.12	0.15	22,27,36,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.